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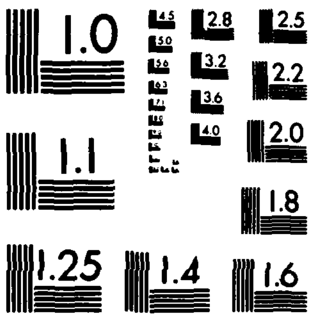
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ATMOSPHERIC TEMPERATURE PROFILES FROM EARTH LIMB

INFRARED MEASUREMENTS

FINAL REPORT

MINIGRANT NO. AFOSR-82-0153

DEPARTMENT OF THE AIR FORCE

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
BOLLING AIR FORCE BASE
WASHINGTON, D.C. 20332

by R.D. HARRIS

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DECEMBER 15, 1982

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FINAL REPORT

Atmospheric Temperature Profiles from Earth Limb Infrared Measurements

Minigrant No. AFOSR-82-0153

Department of the Air Force
Air Force Office of Scientific Research
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December 15, 1982

Submitted by:

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ABSTRACT

This report describes the work accomplished on the retrieval of stratospheric temperature and density profiles from remote earth limb-view infrared radiation measurements. Temperature or density can be retrieved in a routine manner. A model based on two rotational lines of CO_2 was developed to retrieve simultaneously both temperature and density. This model is running on a CRAY-1 Computer but needs additional verification. An investigation of alternative methods to calculate infrared transmittance has showed that an interpolation scheme does work for limb-view geometrics with a subsequent potential savings in computer time of one thousand or better. Though the concept has been proved, the ultimate accuracy of this method has still to be evaluated.

I. INTRODUCTION

This report describes the work that was done on the project "Atmospheric Temperature profiles from Earth Limb Infrared Measurements" for the Air Force Office of Scientific Research, grant no. AFOSR - 82 - 0153. Numerical methods were evolved to utilize remote sensing of the earth limb by infrared radiation measurements in order to determine atmospheric temperature and constituent profiles. These methods are primarily applicable to stratospheric altitudes and for IR measurements such as the AFGL Cryogenic Infrared Radiance Instrumentation for Shuttle (CIRRIS). The work covered two principal areas: 1) An inversion scheme utilizing two rotational lines of CO_2 to retrieve simultaneously temperature and density profiles between about 10 and 65 kms; 2) A method to calculate atmospheric transmittance. This latter task was subdivided into the jobs of developing a very accurate scheme to calculate transmittance of a single rotational line of CO_2 and then proving the feasability of an alternate interpolation scheme to calculate transmittance that would be extremely fast and take less computer time. The details of the inversion algorithm are discussed in the next section. Conclusions and suggestions for further work are given in the third section. Theory covering radiation transport is presented in the appendix.

II. TECHNICAL DISCUSSION

Prior to the start of this work the author had developed two computer codes which would take a set of earth limb IR radiance measurements and calculate a vertical temperature or density profile for the radiating species. (Figure 1 illustrates the limb viewing geometry.) The method was essentially one of choosing some initial profile (temperature or density) and calculating the corresponding limb radiance. Using the difference between the measured and calculated radiances as a modification to the initial profile, a second and hopefully better profile could be obtained.† By successive iterations the first guess

† Chahine M. T., A General Relaxation Method for Inverse Solution of the Full Radiative Transfer Equation, J. Atmos. Sci., 29, pp. 741, 1972

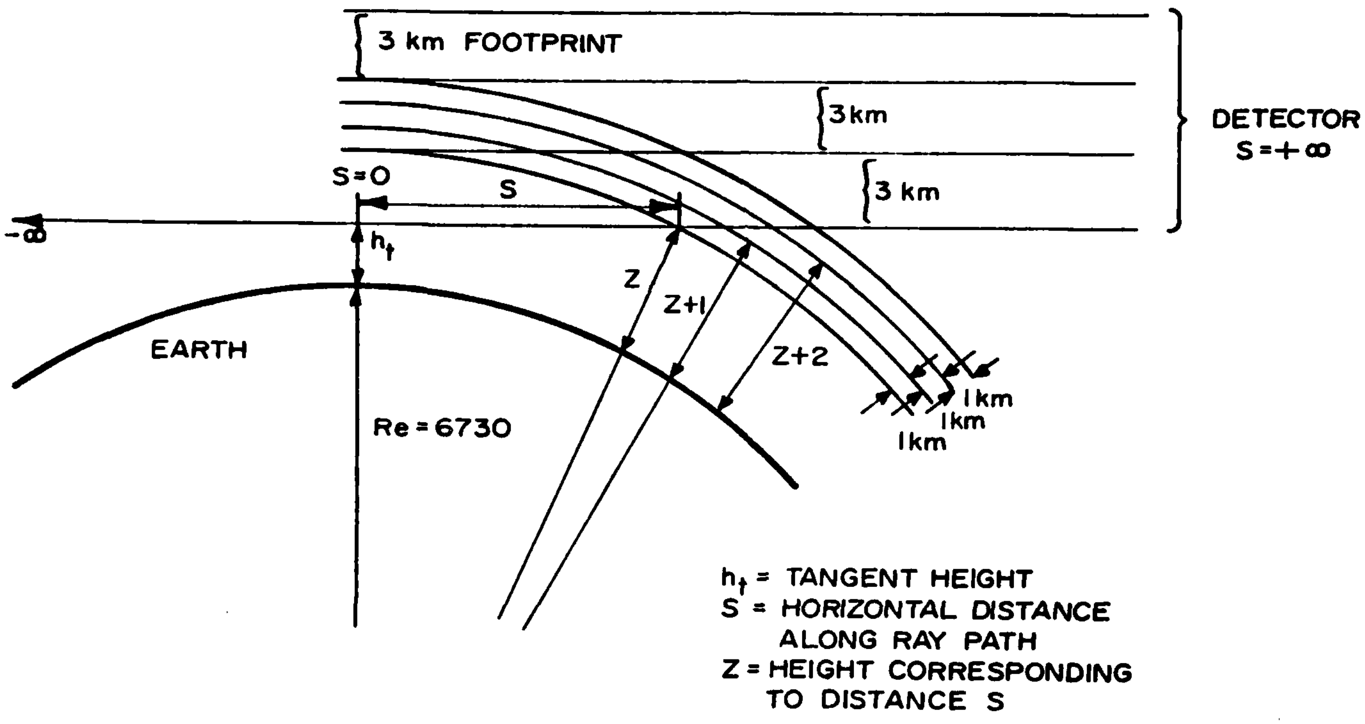


Figure 1. Geometry for Infrared Limb Radiance Inversion Calculations

profile could be reduced to a profile which radiated with the same altitude intensities as those measured. Figure 2 illustrates the convergence process suggested. Thus far we have not used real radiation data since none existed of sufficiently fine resolution. Our "measured" data was actually calculated from a reference atmosphere. For temperature retrieval the density had to be known. For density retrieval the temperature had to be given. The theory of radiation transfer as applied to this remote sensing is given in Appendix A.

Two Line Model

This work of temperature and density retrieval could be directly applicable to the AFGL Cryogenic Infrared Radiance Instrumentation for Shuttle (CIRRIS) data because the wavelength resolutions are about the same. However, with CIRRIS data it will not be possible to specify either a temperature or density for retrieval of the other. What is needed is a method to retrieve both temperature and density simultaneously in a self consistant manner. The problem was attacked by first utilizing the existing computer codes in a push-pull arrangement. A first guess for both temperature and density profiles was used to calculate the radiances for one rotational line. The rotational lines of the CO_2 15μm band were used for this work since the transmittance properties vary from optically thin to very optically opaque. (The whole line was used initially but the transmittance subroutine has now been modified to handle any instrument slit width.) The difference between the calculated and measured radiations was used to modify the initial temperature profile. This new temperature profile and the initial density guess were then used to calculate radiation from the second line. The difference between calculated and measured radiations from this second line was used to modify the density. Both the new density and temperature profiles were now used to calculate a new value of radiation intensity for the first line. Successive radiation calculations back and forth between the lines, together with the successive modifications of the temperature and density profiles was supposed to converge simultaneously the temperature and density profiles to

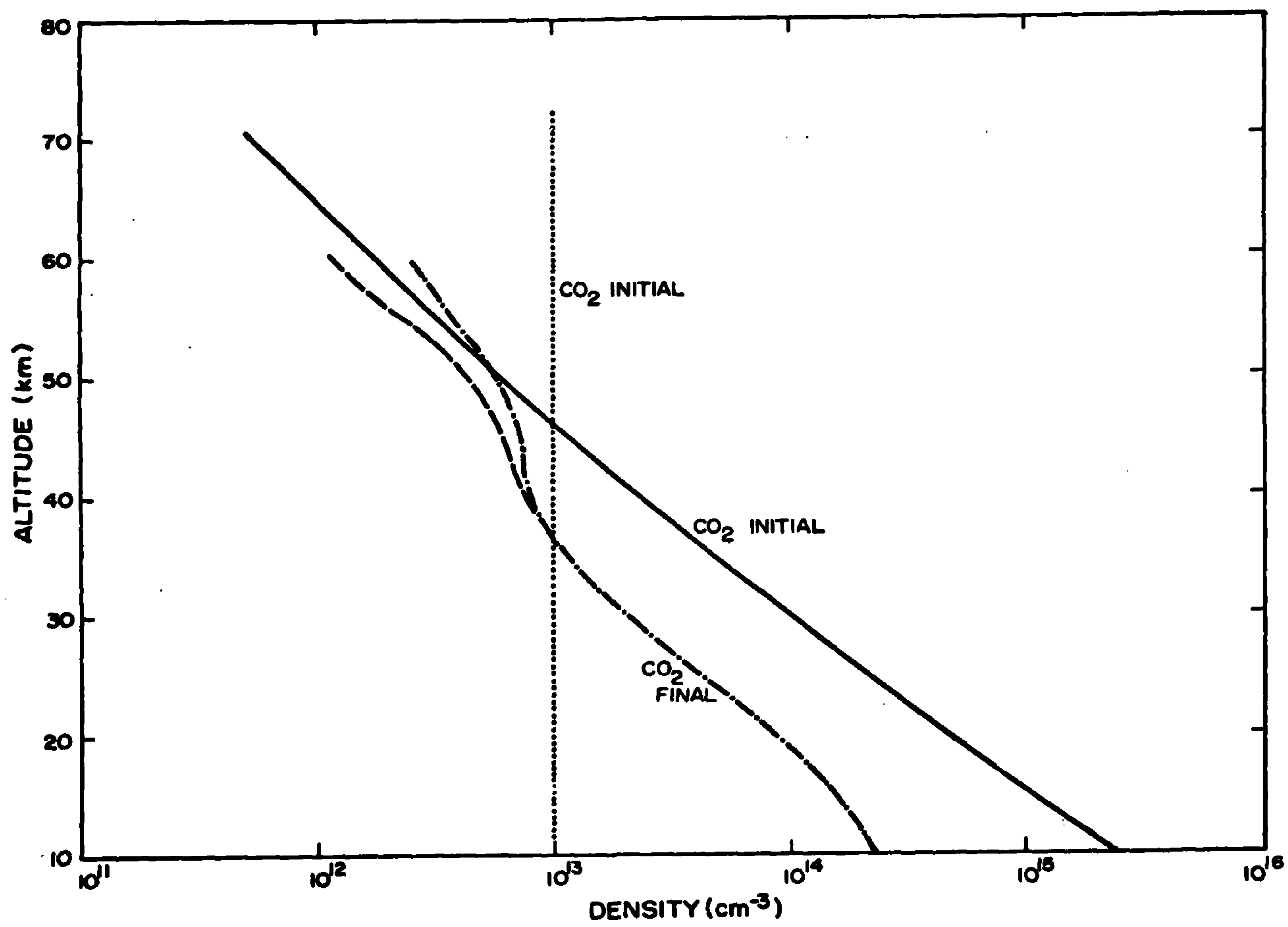


Figure 2. Convergence of Chahine's Relaxation Method for CO_2 Density Retrieval

unique values compatable with the radiation measurements. Unfortunately the method did not perform as anticipated. Temperature and density profiles would indeed converge from their original values to within about 10% of the true values, but then for some reason the temperature and density profiles diverged away from the expected values. This behavior was very unsettling and completely unexpected after the absolute convergence of our earlier results. Because of the large computer costs to run this double line code we were not able to explore or to understand the details of this convergence behavior. We thought that the trouble was caused by inaccuracies in the transmittance calculation. Accordingly a major effort was undertaken to improve the accuracy of the integrated transmittance. Those results are discussed in the next section. At about this time a new two line retrieval scheme was also devised. This scheme is based on the Taylor's series evaluation of a function. If a quantity F is a function of two independent variables x and y, then the Taylor's series expansion is

$$F(x, y) = F(x_o, y_o) + \frac{\partial F}{\partial x}(x - x_o) + \frac{\partial F}{\partial y}(y - y_o) + \sum_{n=2}^{\infty} \frac{1}{n!} \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^n F(x_o, y_o)$$

where $h = x-x_o$ and $k = y-y_o$. If h and k are sufficiently small then the first two terms of the series form a reasonable approximation. Since the limb radiation values are functions of both the temperature and density, the above expression can be used to write

$$\begin{bmatrix} F(T, D) \\ G(T, D) \end{bmatrix} = \begin{bmatrix} F(T_o, D_o) \\ G(T_o, D_o) \end{bmatrix} + \begin{bmatrix} \frac{\partial F}{\partial T} & \frac{\partial F}{\partial D} \\ \frac{\partial G}{\partial T} & \frac{\partial G}{\partial D} \end{bmatrix}_{(T_o, D_o)} \times \begin{bmatrix} T - T_o \\ D - D_o \end{bmatrix}$$

where F and G are the measured radiances of two CO_2 lines, T_o and D_o the first estimate of the temperature and density values which give the trial intensities $F(T_o, D_o)$ and $G(T_o, D_o)$, and T and D are the new temperature and density values which are a linear extrapol tion for e measured intensities F(T, D) and

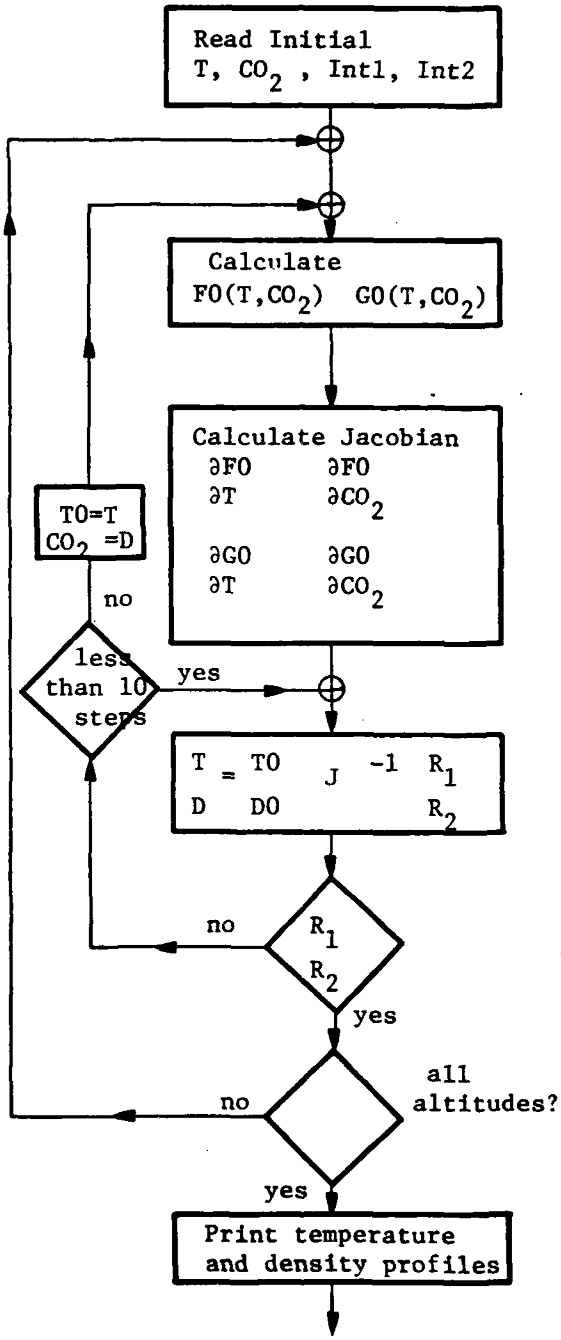
G(T, D). The matrix of partial derivatives is called the Jacobian matrix. Rearranging and multiplying by $[J]^{-1}$ we get the iteration formula.

$$\begin{bmatrix} T \\ D \end{bmatrix} = \begin{bmatrix} T_o \\ D_o \end{bmatrix} + \begin{bmatrix} \frac{\partial F}{\partial T} & \frac{\partial F}{\partial D} \\ \frac{\partial G}{\partial T} & \frac{\partial G}{\partial D} \end{bmatrix}^{-1} \begin{bmatrix} \mathrm{INT1} - F(T_o, D_o) \\ \mathrm{INT2} - G(T_o, D_o) \end{bmatrix}$$

where INT1 and INT2 are the measured IR radiation values. The advantage of this Jacobian matrix method is that the convergence proceeds along the path of maximum descent and does so simultaneously for both temperature and density. The method has been implimented as shown in the flow chart of Figure 3. This method was coded up for the NCAR CRAY-1 Computer, but we ran out of computer funds before the debugging was completed. Discussions with the mathematicians assure us that the scheme will converge provided our initial guesses for T_o and D_o are not too far away from the desired values.

Transmittance Calculations

A calculation of the atmospheric transmittance is necessary whenever a value of the limb radiation is needed. Infrared radiation in the atmosphere is caused by rotational transitions in molecules which have a magnetic moment. Because the molecule has translational kinetic energy and is buffeted by other molecules while in a rotational transition, the absorption - emission line shape i.e. the variation of the radiation intensity versus frequency, changes depending upon its position in the atmosphere. Below 35 km the line is collision broadened, from 40 to 150 km the line is doppler broadened. Since these widths are different one must account for the variable line shape when calculating transmittance. The only method that currently exists to handle the variation in line width is to calculate transmittances at fixed frequency values distributed across the line width. By watching how these individual transmittances vary through the absorbing medium we can then determine the average transmittance characteristic of the entire line. Not only does the line width vary with altitude due to collisions and motion but the amplitude of each line relative to



R_1 = Int1 - FO

R_2 = Int2 - GO

Figure 3. Flow Diagram for Two Line Retrieval Method.

the other lines changes with the change of atmospheric temperature. This is reflected in the changes in the shapes of the P and R branches as a function of temperature.

A Voigt profile, which is a convolution of the Doppler and Lorentz (collision) profiles, was used to describe the smoothly changing line shape. An emperical formula based on the ratio of the Lorentz width to doppler width was devised to specify the effective line width for all altitudes. Forty five points from the line center to half way between lines was considered adequate frequency resolution. Fifteen points were used to specify the core of the line, 10 more points through the wings, and up to 20 more to reach the frequency midway between lines. Forty five points are probably more points than are absolutely necessary but we wanted to be on the conservative side. As the rotational line broadens and flattens out less points are required to accurately specify the shape. Figure 4 is a plot of the transmittance along a limb view line of sight from outside the atmosphere into the tangent altitude for several such optical paths. These curves were all calculated for the J = 26 rotational line of the 15µm CO_2 P branch. Note the complete absorption at the center of the line and the broadening with decreasing altiitude. Also shown are the spacings of the frequency points through the wing of the line. The smooth shape and the coverage afforded by the frequency subdivisions should be accurate enough to handle all the forseeable IR data.

Any infrared sensor has a vertical resolution which depends upon the size of the telescope. For the SPIRE instrument this vertical resolution was an 8 km footprint at the tangent heights. For the CIRRIS instrument and for probably all future data a 3 km footprint size was deemed more satisfactory. It was found that radiation calculations depended critically on the way the density was averaged over the 3 km interval. We finally determined that transmittances should be calculated for each 1 km thick optical path and that a plain average for the three 1 km thick transmittances would be used for the radiation calcula-

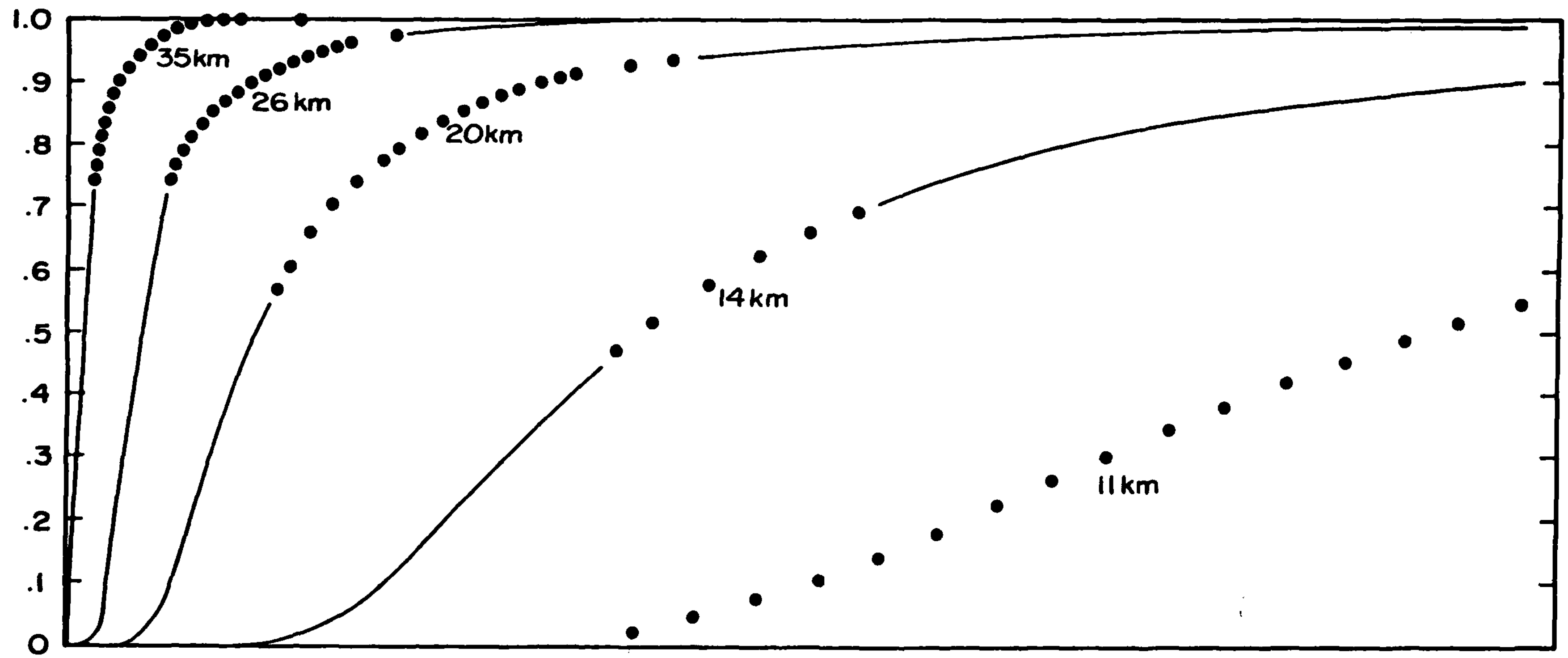


Figure 4. Transmittance at the Indicated Tangent Altitudes Showing the Frequency Distribution and Line Shape

tion. (See Figure 1.) Within each 3 km footprint the density was allowed to have an exponential variation with height. Calculations revealed that radiations from 3 km thick slabs using the average transmittance were almost identical to the sum of the radiations from 3 of the 1 km thick slabs. This must mean that the integrated transmittance over the entire line has a much less extreme variation with density than the individual monochromatic transmittances. An average temperature of the three 1-km slabs was found to be adequate for the calculations. The iteration scheme returns a single temperature and density value for each 3 km slab of atmosphere. Within each 3 km interval along the line of sight the change in transmittance, ΔTr, was found for each individual frequency. The total monochromatic transmittance at frequency ν_j from level i to the top of the atmosphere could then be written.

$$Tr_{i+1}(\nu_j) = \Delta Tr_i(\nu_j)\, Tr_i(\nu_j)$$

Since the line width changes with altitude, the previous values of transmittance $Tr_i(\nu_k)$ had to be interpolated to the new frequencies ν_j. The integrated transmittance was then found by integrating $Tr_{i+1}(\nu_j)$ over frequency. The integrated transmittance was given numerically by

$$Tr_{i+1} = \sum_{j=1}^{45} Tr_{i+1}(\nu_j)\, \Delta\nu_j$$

The variation of transmittance for the J = 26 rotational line of the CO_2 15μm P branch is plotted for eight different tangent altitudes in Figure 5. Obviously the total transmittance increases for increased depth into the atmosphere. The radiation leaving the atmosphere along the i^{th} tangent line of sight is found by the formula

$$R_i = \int_0^{Tr_i} B(T)\, dTr\,(T, CO_2, s)$$

where B is the Planck Function and the transmittance Tr is a function of temperature, density and obviously position along the line of sight. According to this expression the maximum radiation comes from the altitudes where the trans-

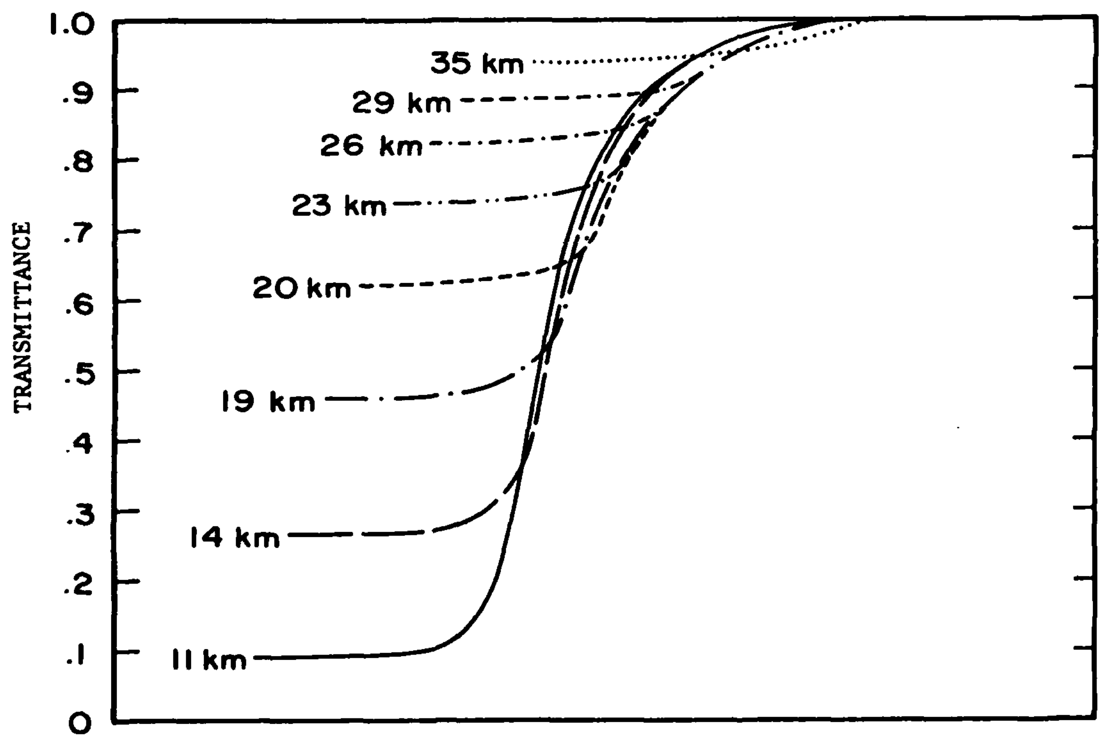


Figure 5. Integrated Transmittance for the J=26 Rotational Line of CO_2 15 μm band P branch and for the Tangent Heights Shown.

mittance has the greatest change. Figure 6 is a plot of transmittance for a number of different rotational lines and different tangent altitudes. It can be seen that the radiation at different lines comes from different altitudes. For the simultaneous temperature and density retrieval, we chose the $J = 26$ line which has good variation between 11 and 65 kms for one of the lines. The other line was a composite of the $J = 2$ and $J = 31$ lines. Between 11 - 17 km the $J = 31$ line gave adequate change in transmittance, while the $J = 2$ line was satisfactory between 20 and 65 km.

The method for calculating transmittances as briefly described above is accurate but takes an excessive amount of computer time. For real data sets such as will be obtained from the CIRRIS experiment a much faster and cheaper scheme must be found to calculate transmittance. We believe such a scheme is afforded by the McMillin† technique.

McMillin Calculation of Transmittance

McMillin's method was designed and has been successfully used for inversion of data from vertically downward looking instruments which have a band width of many rotational lines and the band includes radiation from several different species. For the limb viewing geometry we desire a calculation of transmittance over a bandwidth of only one rotation line and considering only one species. The transmittance is calculated in steps along the line of sight path using the expression

$$Tr_i = \Delta Tr_i \; Tr_{i-1}$$

where the transmittance is given by the expansion

$$\Delta Tr_i = \sum_{j=1}^{12} c_{ij} \; x_{ij}$$

† McMillin, L. M., H. F. Fleming and M. L. Hill, Atmospheric transmittance of an absorbing gas. 3: A computationally fast and accurate tranmittance model for absorbing gases with variable mixing ratios, Appl. Optics, 18, pp. 1600, 1979.

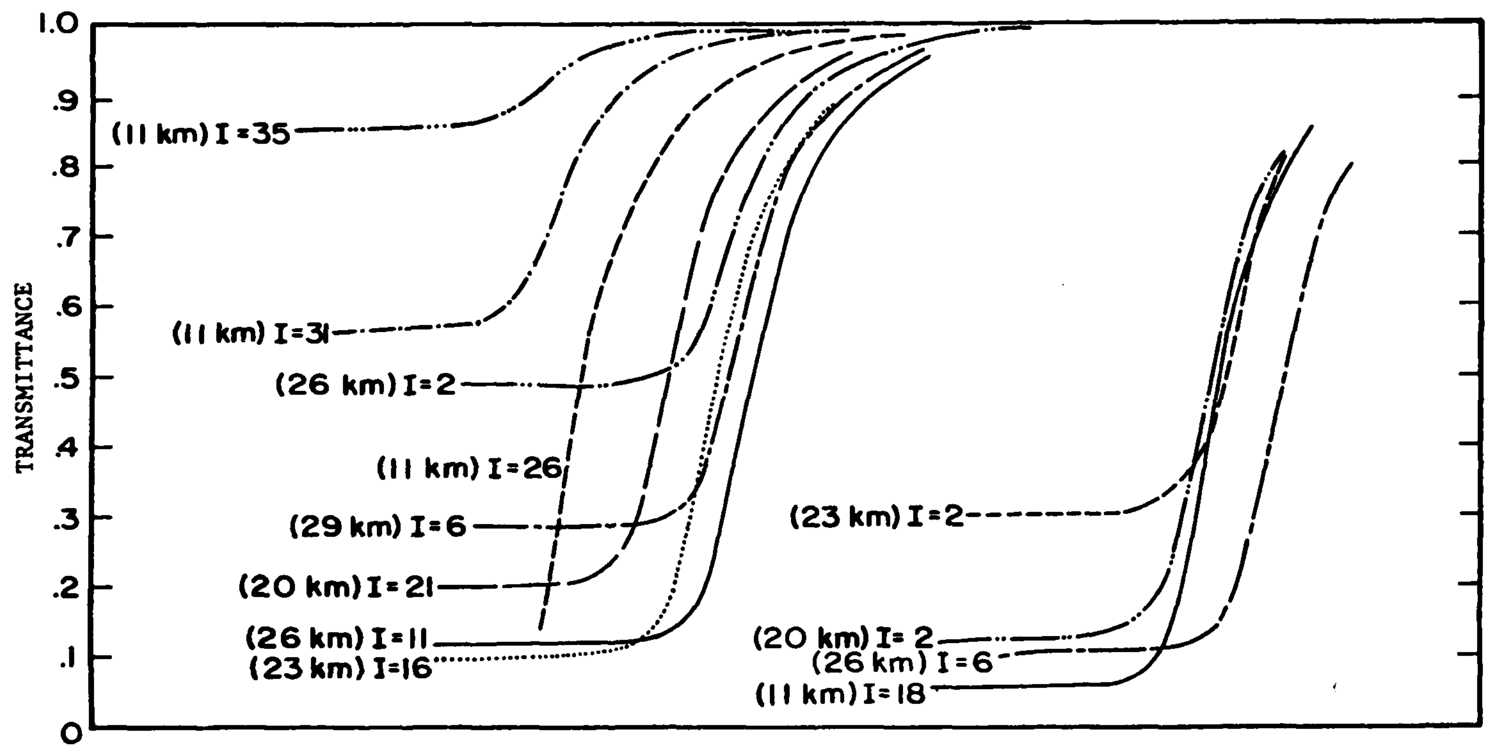


Figure 6. Variation in Transmittances for the CO_2 Rotational Lines and Tangent Altitudes Shown

with

$$x_{i1} = 1 \qquad x_{i2} = \Delta T_i$$

$$x_{i3} = \Delta p_i \qquad x_{i4} = \Delta T^2$$

$$x_{i5} = \Delta T_i \Delta p_i \qquad x_{i6} = \Delta p_i^{\,2}$$

$$x_{i7} = \Delta T_i \Delta p_i^{\,2} \qquad x_{i8} = \Delta T_i^{*}$$

$$x_{i9} = \Delta p_i^{*} \qquad x_{i10} = \Delta T_i^{**}$$

$$x_{i11} = \Delta p_i^{**} \qquad x_{i12} = \Delta T_i^{***}$$

$$\Delta T_i = T_i - \hat{T}_i$$

$$\Delta p_i = p_i - \hat{p}_i$$

The hat ^ over T and p refers to reference atmosphere values. In the calculation a reference atmosphere must be chosen with temperature profile $\hat{T}$ and pressure profile $\hat{p}$. The total column density for the reference atmosphere is larger than for any other atmosphere for which the transmittance is to be calculated. The independent variable in these expressions is column density along the path

$$\tau_i = \int \sigma_o f_v n(z) ds$$

which is also called the optical depth in (1) of the appendix. The various starred quantities along the path are weighted averages defined by

$$\Delta T_i^{*} = \int_o^{\tau_i} \Delta T d\tau \Big/ \int_o^{\tau_i} d\tau$$

$$\Delta p_i^{*} = \int_o^{\tau_i} \Delta p d\tau \Big/ \int_o^{\tau_i} d\tau$$

$$\Delta T_i^{**} = \int_o^{\tau_i} \tau \Delta T d\tau \Big/ \int_o^{\tau_i} d\tau$$

$$\Delta p_i^{**} = \int_o^{\tau_i} \tau \Delta p \Big/ \int_o^{\tau_i} d\tau$$

$$\Delta T_i^{***} = \int_o^{\tau_i} n \Delta T \Big/ \int_o^{\tau_i} d\tau$$

$$\Delta T = T - \hat{T}$$

$$\Delta p = p - \hat{p}$$

In order to use the transmittance as given by the series expansion it is necessary to have ΔTr_i small. McMillin suggested that 100 steps of about equal transmittance difference should give good accuracy. To generate the coefficient C_{ij}, a number of model atmospheres must be chosen and used as the basis atmospheres. The basis must contain more than 12 different models and the models should be chosen to cover as wide a range of parameters as is expected in the transmittance calculations. These basis models are used to generate transmittance values at each of the reference column densities τ_i. The C_{ij}'s are found which give the best mean square fit to these transmittance of the basis atmospheres. The exception to this mean square fit is C_{i1} which is chosen so that

$$C_{i1} = \frac{\hat{Tr}_i}{\hat{Tr}_{i-1}}$$

Our test of the McMillin calculation used the J = 10 rotational line of the P branch of the 15µm band of CO_2. The model atmospheres for the basis atmosphere were generated mathematically using the hydrostatic equation, constant CO_2 mixing ratio (3.16×10^{-4}), and various assumed temperature profiles. Some of these profiles are shown in Figure 7. All the temperature profiles fell within $\pm 10^{\circ}$K of the solid line profile of Figure 7. A total of nine different profiles were used to generate nine different atmospheres. Each of these model atmospheres was used to generate transmittance curves, such as shown in Figure 4, for each tangent height. Actually there were 17 tangent heights of 3 km slabs between 12 km and 60 km. The reference model atmosphere was chosen from the basis atmospheres to be that atmosphere with the maximum column density. The model atmosphere to the extreme right of Figure 7 was the reference atmosphere for these calculations. Using this atmosphere and the smallest tangent height, a calculation of transmittance vs. column density was made. The reference column density was found by dividing the total transmittance into 100 equal multipli-

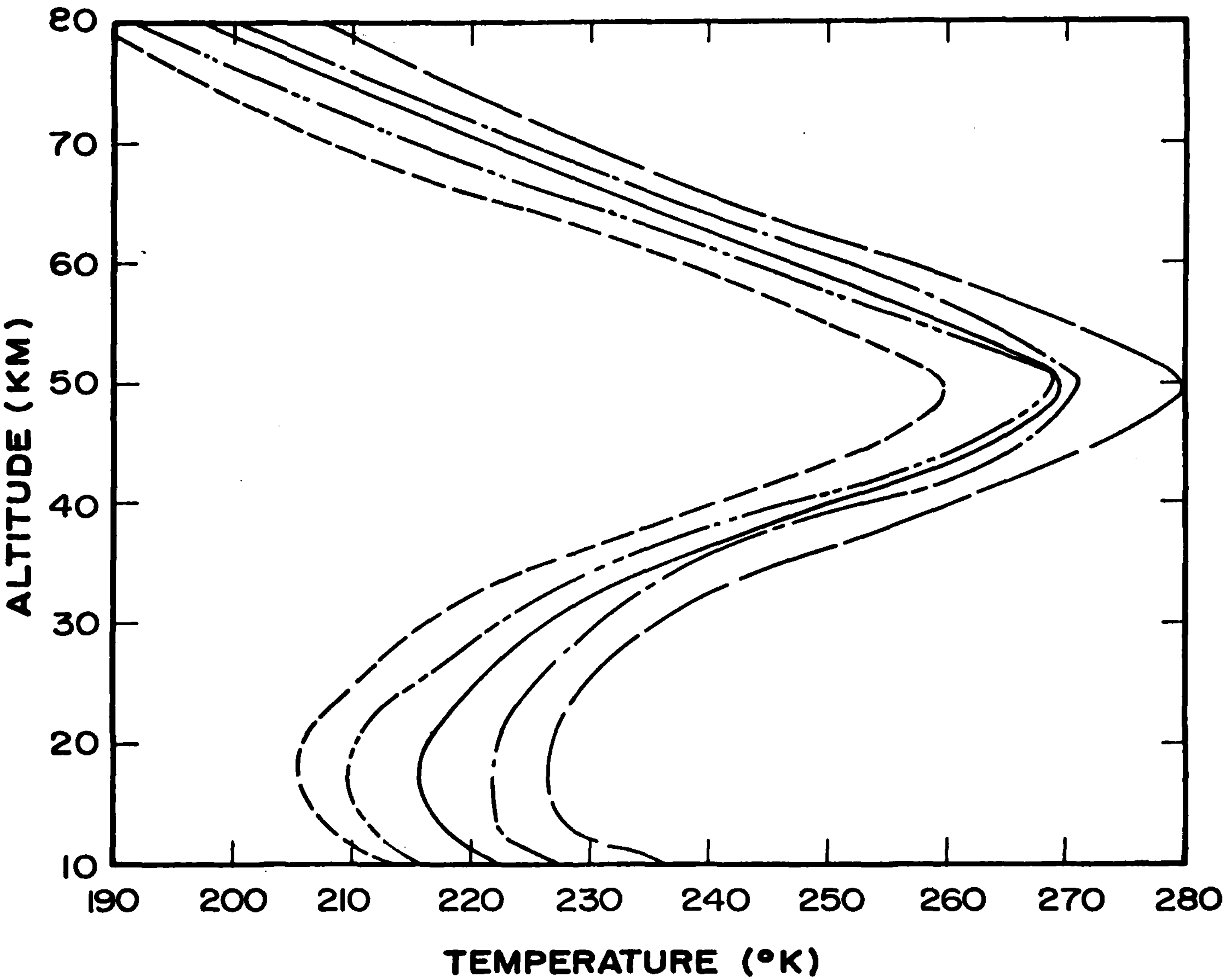


Figure 7. Temperature Profiles of Basis Atmospheres used for McMillin Transmittance Calculations.

cative steps i.e. making the ΔTr_i's in the formula

$$Tr_i = Tr_{i-1} \Delta Tr_i$$

all equal with Tr_{100} equal to the maximum transmittance calculated. The positions corresponding to this set of reference $\hat{Tr}_i$'s also specify a corresponding set of τ_i's. (The τ_i's imply a set of reference pressure $\hat{p}_i$ and temperature $\hat{T}_i$.) The $\hat{Tr}_i$'s can be used immediately to generate $C_{i1} = \hat{Tr}_i/\hat{Tr}_{i-1}$. To find the other C_{ij}'s we calculate the transmittance, the difference between temperatures $\Delta T_i = T_i - \hat{T}_i$, and the pressure difference $\Delta p_i = p_i - \hat{p}_i$, at all τ_i's for each of the other atmospheres and at all tangent heights. This gives us a set of ΔTr_i at each τ_i which then allows a mean square fit to evaluate the C_{ij}'s.

One problem with this fitting technique occurs because the different tangent height calculations for the same model atmosphere differ only significantly near the tangent point. This causes an abnormal weighting of the least square fit of ΔTr_i. To alleviate this problem, if the set of ΔTr_i's at some τ_i contain a number of ΔTr_i's which are identical, only two of the identical values are used in the fit.

With the C_{ij}'s calculated, it was now time to evaluate the McMillin expansion. Accordingly a test model atmosphere, shown as the dotted profile in Figure 8, was devised to lie within the limits of the basis atmospheres but not equal to any of them. The exact tranmittance was calculated with the 45 point routine described earler. The McMillin transmittances were found by substituting the values of temperature from Figure 8 at the reference τ_i's into ΔT_i and the pressure into Δp_i. The corresponding values of x_{ij} were then found at each of the 100 positions. Finally the expansion

$$\Delta Tr_i = \sum_{j=1}^{12} C_{ij} x_{ij}$$

was evaluated and the transmittances calculated by

$$Tr_i = Tr_{i-1} \Delta Tr_i$$

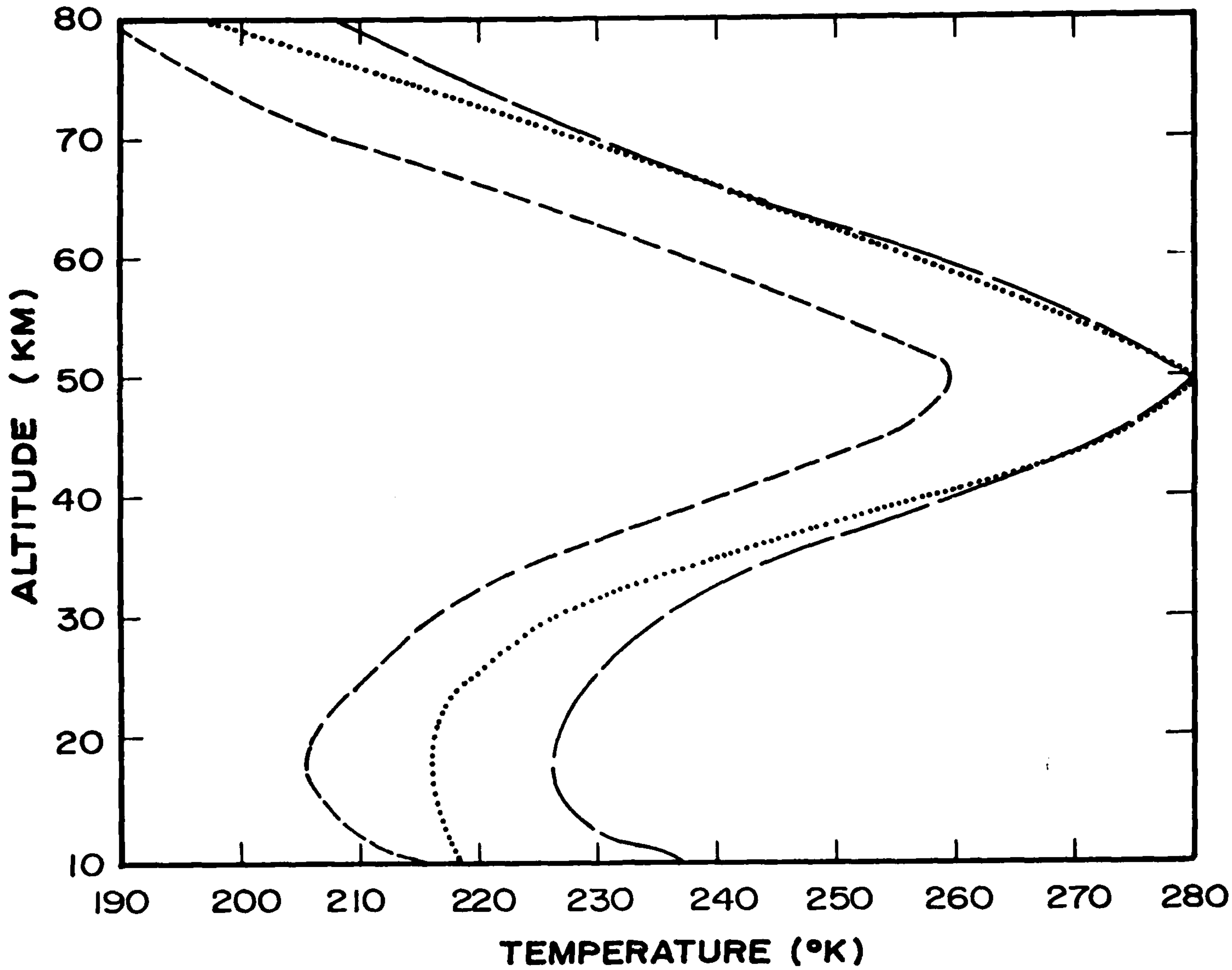


Figure 8. Model Atmosphere to Test McMillin Expansion for Transmittance.

Table I shows a comparison of the exact transmittance and the transmittance calculated from the McMillin formulas. Also shown is the absolute error. Note the absolute errors are very small, but they are also rather difficult to interpret. One possible way of determining their significance is to compare them with the change in transmittance caused by a change in temperature (the sensitivity of transmittance to temperature). This estimate of sensitivity is also shown at steps 25 and 40 along the line of sight.

The calculations of transmittance for the test model atmosphere was found to give poor results beyond step 40. This was caused by too few different atmospheres, in our case only 9, used in the determination of the C_{ij}'s at large τ_i's. At least 12 different ΔTr_i's at every τ_i are needed to make a good mean square fit. With 9 model atmospheres and 17 tangent heights this is easy for the case of small τ_i's but not large τ_i's since only one tangent height produces the largest τ_i. A basis with perhaps 20 model atmospheres should correct this problem.

Note that the McMillin formulation that has been discussed above attempts to fit the transmittance calculation at all tangent heights with one set of coefficients C_{ij}. This was only partially successful. At the higher tangent heights the column densities are such that even the first step of transmittance is not seen along the entire path. Perhaps the calculations for different tangent heights will have to be handled with different sets of coefficients based on different column density steps τ_i. It does look as if a group of tangent heights can be handled with the same set of column density steps τ_i and coefficients C_{ij}. Even if a set of coefficients were needed for each tangent altitude, the computer storage requirements would be small enough to fit on a VAX type computer.

TABLE I

Comparison of Exact and McMillin Calculation

of Transmittance (Tr_i) Tangent Height -- 13 km.

Step (i)	(Tr_i) Exact	(Tr_i) McMillin	Abs Error	Abs Sensitivity (per °K)
5	0.96849	0.96843	0.00006	
10	0.93732	0.93776	0.00044	
15	0.90870	0.90803	0.00067	
20	0.87969	0.87901	0.00068	.00017
25	0.85506	0.85397	0.00109	
30	0.82840	0.82803	0.00037	
35	0.79827	0.79809	0.00018	
40	0.74487	0.74781	0.00594	.0010

III. CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

A model of infrared radiation from CO_2 has been developed that is applicable to earth limb radiation from the stratosphere. The kernel of this model is a numerical code to calculate the integrated transmittance of a single rotational line. (However, a modification has been made so that any fraction of the rotational line can also be handled.) Using a non-linear iteration process it has been shown that temperature or CO_2 density profiles in the stratosphere can be found from IR limb radiation measurements. A numerical code has been developed to utilize two rotational lines of CO_2 to retrieve both temperature and CO_2 density simultaneously. This code is running but needs verification. If CO_2 is well mixed in the atmosphere a simultanious retrieval of temperature and density will yield the atmospheric pressure profile and allow numerous densities of other IR active species to be deduced.

A computationally fast method for evaluation of transmittance has also been studied. This interpolation scheme, first proposed by McMillin for vertical looking sensors, has been reformulated for limb viewing and run with a subminimum number of basis atmosphere models to prove out the concept. Results were very encouraging. An evaluation of this technique with 12 - 20 model atmospheres should be made to see if one set of expansion coefficients, which only have to be calculated once for each sensor and each radiation band, can be used for the entire atmosphere or the other extreme of a set of coefficients for each tangent altitude. The ultimate accuracy that can be obtained in a retrieval scheme in degrees of temperature or percent of density using this method to calculate transmittance will undoubtely depend on the number of sets of expansion coefficients.

With some additional work two numerical codes could be developed to retrieve atmospheric temperature and pressure, and minor species concentration profiles from the stratosphere. These codes would include the McMillin method of calculating transmittance, which is such an improvement in computational speed

that perhaps the retrieval code could operate in real observing time. (Development and verification of the codes would need to be done on a large computer but the final versions could easily run on a VAX sized machine.) If these retrieval codes were tailored to the band pass and field of view of the CIRRIS instrument, routine profiles of minor and trace gases in the stratosphere and on a gobal scale could be obtained from future CIRRIS missions.

APPENDIX A

The geometry of the limb radiance calculations is shown in Figure 1. The atmosphere is assumed to be layered and spherically symmetric. Temperature, pressure, and constituent densities are specified each kilometer from 100 km down to the surface. The horizontal distance from the tangent point to some point along the ray path, s, is related to altitude, z, as indicated in Figure 1.

The "optical" depth is found by the expression:

$$\tau(\nu, s) = \int_s^\infty \sigma_o \, n(s) \, f_v(x, y) \, ds \tag{1}$$

where σ_o = absorption cross section at line center

ν_o = wave number at line center

ν = wavenumber (frequency)

$x = (\nu - \nu_o)\alpha_D$

α_D = doppler half width

$y = \alpha_L/\alpha_D$

α_L = Lorentz half width

n = absorbing species density

and f_v is the Voigt line shape function.

The transmission from an element at s to the detector, which is assumed to be at $s = \infty$, is

$$Tr_\nu(s) = e^{-\tau(\nu, s)} \tag{2}$$

The mean transmission over the wave number interval $\nu_2 - \nu_1$ for a rectangular slit function is

$$\langle Tr(s) \rangle = \int_{\nu_1}^{\nu_2} Tr_\nu(s) \, d\nu/(\nu_2 - \nu_1)$$

The spectral radiance at the detector is

$$I(\nu) = \int_{-\infty}^{\infty} \phi(\nu - \nu_o) \, B(\nu, T(z)) \frac{\partial Tr_\nu(s)}{\partial s} ds$$

where B is the Planck blackbody function and $\phi(\nu - \nu_o)$ is the instrument slit function. For a single line the integrated radiance is

$$I = \int_{\nu_1}^{\nu_2} d\nu \int_{-\infty}^{\infty} \phi(\nu - \nu_o)\, B(\nu,\, T(z))\, \frac{\partial Tr\nu}{\partial s}\, ds$$

Since the frequency variation of the Planck function is small for a single line $B(\nu, T(z)) \sim B(\nu_o, T(z))$ and we can write

$$I = \int_{\nu_1}^{\nu_2} \phi(\nu - \nu_o) d\nu \int_{-\infty}^{\infty} B(\nu_o,\, T(z))\, \frac{\partial Tr}{\partial s}\, ds$$

where Tr is the average transmission over the line. Since all measurements will have at least a 3 km vertical footprint we must also integrate over the vertical field of view.

$$\bar{I} = \int_{\nu_1}^{\nu_2} \phi(\nu - \nu_o) d\nu \int_{\Delta h_t} dh_t \int_{-\infty}^{\infty} B(\nu_o,\, T(z))\, \frac{\partial Tr}{\partial s}\, ds\, dh_t$$

But we again assume $B(\nu_o, T(z))$ is relatively constant over Δh_t, or at least can be represented by some average, so

$$\bar{I} = \int_{\nu_1}^{\nu_2} \phi(\nu - \nu_o) d\nu \Delta h_t \int_{-\infty}^{\infty} B(\nu_o,\, T(z))\, \frac{\partial}{\partial s} \left[\frac{1}{\Delta h_t} \int_{\Delta h_t} Tr\, dh_t \right] ds$$

The expression in the brackets is just the average transmission over the vertical footprint and over the entire rotational line. If we give it the symbol $\overline{Tr}$ then

$$\bar{I} = \int_{\nu_1}^{\nu_2} \phi(\nu - \nu_o) d\nu\; \Delta h_t \int_{-\infty}^{\infty} B(\nu,\, T(z))\, \frac{\partial \overline{Tr}}{\partial s}\, ds$$

Note that the radiance depends not on the transmission function but rather on the derivative with respect to distance along the line of sight of the transmission.

Chahine suggested a technique for determining temperature or constituent

densities with a vertical looking instrument which looks down into the atmosphere and scans the wavenumber. The limb scan problem is different in that we have a set of equations (for a single line)

$$I_i = \int_{-\infty}^{\infty} B(T(z)) \frac{\partial \overline{Tr}_i}{\partial s} ds \tag{4}$$

where the index i has been added to equation (3) to refer to the different tangent height measurements. Some of the constants are absorbed in $\overline{Tr}_i$. This is not a single integral equation but a set of equations, one equation for each tangent height. Suppose we know n(z) and wish to find the temperature from (4). The method of solution is to iterate the temperature profile in the equation

$$I_i^m = \int_{-\infty}^{\infty} B(T^m (z)) \frac{\partial \overline{Tr}_i}{\partial s} ds \tag{5}$$

until the set of residuals

$$R^m = \frac{\tilde{I}_i - I_i^m}{\tilde{I}_i}$$

where $\tilde{I}_i$ is the measured intensity at tangent altitudes i approach a stable set of minimum values. The technique of iteration is to satisfy equation (4) at each tangent altitude separately. Thus if we multiply the right side of (5) by $\tilde{I}_i/I_i^m$

$$\tilde{I}_i = \frac{\tilde{I}_i}{I_i^m} \int_{\infty}^{\infty} B(T^m (z)) \frac{\partial \overline{Tr}_i}{\partial s} ds$$

and the temperature is iterated by the recursive formula

$$B(T^{m+1}(z)) = \frac{\tilde{I}_i}{I_i^m} B(T^m (z)) \tag{6}$$

Equation (6) is a set of recursive equations giving new temperature profiles T^{m+1} in terms of old profiles T^m. We make the solution of these equations unique by using the equation for the ith tangent altitude to find the new temperature

at that altitude in terms of the old temperature at that altitude.

$$B(T^{m+1}(z_i)) = B(T^{m}(z_i)) \frac{\bar{I}_i}{I_i^{m}}$$

where z_i is the ith tangent altitude. Now we can find a new set of radiances I^{m+1} using the new temperatures (equation 5). The process continues until the residuals become constant and hopefully small.

To solve for densities it is convenient to integrate (4) by parts giving

$$\bar{I}_i = Tr_i(n(\infty))B(T(\infty)) - Tr_i(n(-\infty))B(T(-\infty)) + \int_{-\infty}^{\infty} Tr_i(n(z)) \frac{\partial B(z)}{\partial s}\, ds \quad (7)$$

where we have shown Tr_i as an explicit function of constituent density n(z). Assume the temperature profile is known or has been determined from another measurement. The problem is formulated in much the same way as the temperature inversion problem. The density is iterated in the equations

$$I_i^{(j)} = Tr(n^{j}(\infty))B(T(\infty)) - Tr(n^{j}(-\infty))B(T(-\infty)) + \int_{-\infty}^{\infty} Tr(n^{(j)}(z))\frac{\partial B}{\partial s}\, ds \quad (8)$$

until the set of residuals

$$r_i^{m} = \bar{I}_i - I_i^{m}$$

approach a set of minima. To find the new density profile in terms of an old profile the recursive relations are written as

$$n^{m+1}(z_i) = \alpha_i^{m}\, n(z_i) \quad (9)$$

and the α_i are found by some nonlinear technique. One technique is to use Newton's method and consider the iteration one tangent altitude at a time, i.e.

$$n^{m+1}(z_i) = \alpha_i^{m}\, n(z)$$

We start with $\alpha_i^{1} = 1$ and calculate the corresponding I_i^{1}, and r_i^{1}. Then we assume a second set of α_i, say $\alpha_i^{2} = \bar{I}_i/I_i^{1}$ and calculate the corresponding I_i^{2} and r_i^{2}. Now in the linear approximation r_i^{3} will be zero if α_i^{3} is given by

$$\alpha_i^m = \alpha_i^{m-2} - r_i^{m-2} \left\{ \frac{\alpha_i^{m-2} - \alpha_i^{m-1}}{r_i^{m-2} - r_i^{m-1}} \right\}$$

This formula can be used for further iterations using for r_i^{m-2} the minimum of all previous r_i^m and the corresponding α_i^m for α_i^{m-2}. The process terminates when the set of r_i^m are minimum. Having found a set of α_i we now return to equation (9) and find a new $n(z)$ and repeat until convergence is obtained in the sense the α_i all approach one.

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5